

# ON THE EXISTENCE OF ENERGY-PRESERVING SYMPLECTIC INTEGRATORS BASED UPON GAUSS COLLOCATION FORMULAE \*

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**Abstract.** We introduce a new family of symplectic integrators depending on a real parameter  $\alpha$ . For  $\alpha = 0$ , the corresponding method in the family becomes the classical Gauss collocation formula of order  $2s$ , where  $s$  denotes the number of the internal stages. For any given non-null  $\alpha$ , the corresponding method remains symplectic and has order  $2s - 2$ : hence it may be interpreted as a  $O(h^{2s-2})$  (symplectic) perturbation of the Gauss method. Under suitable assumptions, we show that the parameter  $\alpha$  may be properly tuned, at each step of the integration procedure, so as to guarantee energy conservation in the numerical solution. The resulting method shares the same order  $2s$  as the generating Gauss formula.

**Key words.** Hamiltonian systems, collocation Runge-Kutta methods, symplectic integrators, energy-preserving methods.

**AMS subject classifications.** 65P10, 65L05

**1. Introduction.** We consider canonical Hamiltonian systems in the form

$$\begin{cases} \dot{y} = J \nabla H(y) \equiv f(y), \\ y(t_0) = y_0 \in \mathbb{R}^{2m}, \end{cases} \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \in \mathbb{R}^{2m \times 2m}, \quad (1.1)$$

( $I$  is the identity matrix of dimension  $m$ ). Regarding its numerical integration, two main lines of investigation may be traced, having as objective the definition and the study of symplectic methods and energy-conserving methods, respectively. In fact, symplecticity and the conservation of the energy function are the most relevant features characterizing a Hamiltonian system.

From the very beginning of this research activity, high order symplectic formulae were already available within the class of Runge-Kutta methods, the Gauss collocation formulae being one noticeable example. One important implication of symplecticity of the discrete flow is the conservation of quadratic invariants. This circumstance makes the symplecticity property of a method particularly appealing in the numerical simulation of isolated mechanical systems in the form (1.1), since it provides a precise conservation of the total angular momentum during the time evolution of the state vector. As a further positive consequence, a symplectic method also conserves quadratic Hamiltonian functions (see the monographs [12, 18, 21] for a detailed analysis of symplectic methods).

On the other hand, excluding the quadratic case, energy-conserving methods were initially not known within the class of classical methods and as a matter of facts, among the first attempts to address this issue, projection and symmetric projection techniques were coupled to classical non-conservative schemes in order to impose the numerical solution to lie in a proper manifold representing a first integral of the original system (see [13, Sect. VII.2], [1, 11] and [12, Sect. V.4.1]).

A completely new approach is represented by *discrete gradient methods* which are based upon

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the definition of a discrete counterpart of the gradient operator so that energy conservation of the numerical solution is guaranteed at each step and whatever the choice of the stepsize of integration (see [9, 20]).

More recently, the conservation of energy has been approached by means of the definition of the *discrete line integral*, in a series of papers (such as [15, 16]), leading to the definition of *Hamiltonian Boundary Value Methods (HBVMs)* (see for example [3, 4]). These are a class of methods able to preserve, in the discrete solution, polynomial Hamiltonians of arbitrarily high degree (and hence, a *practical* conservation of any sufficiently differentiable Hamiltonian)<sup>1</sup>. Such methods admit a Runge-Kutta formulation which reveals their close relationship with classical collocation formulae [5]. An infinity extension of HBVMs has also been proposed in [10, 4].

Attempts to incorporate both symplecticity and energy conservation into the numerical method will clash with two non-existence results. The first [8] refers to non-integrable systems, that is systems that do not admit other independent first integrals different from the Hamiltonian function itself. According to the authors' words, it states that

*If [the method] is symplectic, and conserved  $H$  exactly, then it is the time advance map for the exact Hamiltonian system up to a reparametrization of time.*

The second negative result [7] refers to B-series symplectic methods applied to general (not necessarily non-integrable) Hamiltonian systems:

*The only symplectic method (as B-series) that conserves the Hamiltonian for arbitrary  $H(y)$  is the exact flow of the differential equation.*

The aim of the present work is to devise methods of any high order that, in a sense that will be specified below and under suitable conditions, may share both features. More precisely, we will begin with introducing a family of one-step methods

$$y_1(\alpha) = \Phi_h(y_0, \alpha) \tag{1.2}$$

( $h$  is the stepsize of integration), depending on a real parameter  $\alpha$ , with the following specifics:

1. for any fixed choice of  $\alpha \neq 0$ , the corresponding method is a symplectic Runge-Kutta method with  $s$  stages and of order  $2s - 2$ ;
2. for  $\alpha = 0$  one gets the Gauss collocation method (of order  $2s$ );
3. for any choice of  $y_0$  and in a given range of the stepsize  $h$ , there exists a value of the parameter, say  $\alpha^*$ , depending on  $y_0$  and  $h$ , such that  $H(y_1) = H(y_0)$  (energy conservation).

As the parameter  $\alpha$  ranges in a small interval centered at zero, the value of the numerical Hamiltonian function  $H(y_1)$  will match  $H(y(t_0 + h))$ , thus leading to energy conservation. This result, which will be formally proved in Section 4, is formalized as follows:

*Under suitable assumptions, there exists a real sequence  $\{\alpha_k\}$  such that the numerical solution defined by  $y_{k+1} = \Phi_h(y_k, \alpha_k)$ , with  $y_0$  defined in (1.1), satisfies  $H(y_k) = H(y_0)$ .*

To clarify this statement and how it relates to the above non-existence results, we emphasize that the energy conservation property only applies to the specific numerical orbit  $\{y_k\}$  that the method generates, starting from the initial value  $y_0$  and with stepsize  $h$ . For example, let us consider the very first step and assume the existence of a value  $\alpha = \alpha_0$ , in order to enforce the energy conservation

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<sup>1</sup>We refer the reader to [2] for a complete documentation on HBVMs.

between the two state vectors  $y_0$  and  $y_1$ , as indicated at item 3 above. If  $\alpha_0$  is maintained constant, the map  $y \mapsto \Phi_h(y, \alpha_0)$  is symplectic and, by definition, assures the energy conservation condition  $H(y_1) = H(y_0)$ . However, it would fail to provide a conservation of the Hamiltonian function if we changed the initial condition  $y_0$  or the stepsize  $h$ : in general, for any  $\hat{y}_0 \neq y_0$ , we would obtain  $H(\Phi_h(\hat{y}_0, \alpha_0)) \neq H(y_0)$ . Thus, the energy conservation property we are going to discuss weakens the standard energy conservation condition mentioned in the two non-existence results stated above and hence, by no means, the new methods are meant to produce a counterexample of these statements.

The paper is organized as follows. In the next section we report the definition of the methods while in Section 3 we show their geometrical link with Gauss collocation formulae. In Section 4 we face the problem from a theoretical viewpoint and give some existence results that aim to explain the energy-preserving property of the new methods. In Section 5 we report a few tests that give a clear numerical evidence that a change in sign of the function  $g(\alpha) = H(y_1(\alpha)) - H(y_0)$  does indeed occur along the integration procedure.

**2. Definition of the methods.** Let  $c_1 < c_2 < \dots < c_s$  and  $b_1, \dots, b_s$  be the abscissae and the weights of the Gauss-Legendre quadrature formula in the interval  $[0, 1]$ . We consider the Legendre polynomials  $P_j(\tau)$ , of degree  $j - 1$  for  $j = 1, \dots, s$ , shifted and normalized in the interval  $[0, 1]$ , that is

$$\int_0^1 P_i(\tau) P_j(\tau) d\tau = \delta_{ij}, \quad i, j = 1, \dots, s, \quad (2.1)$$

( $\delta_{ij}$  is the Kronecker symbol), and the matrix

$$\mathcal{P} = \begin{pmatrix} P_1(c_1) & P_2(c_1) & \cdots & P_s(c_1) \\ P_1(c_2) & P_2(c_2) & \cdots & P_s(c_2) \\ \vdots & \vdots & & \vdots \\ P_1(c_s) & P_2(c_s) & \cdots & P_s(c_s) \end{pmatrix}_{s \times s}. \quad (2.2)$$

Our starting point is the following decomposition of the Butcher array  $A$  of the Gauss method of order  $2s$  (see [13, Theorem 5.6]):

$$A = \mathcal{P} X_s \mathcal{P}^{-1}, \quad (2.3)$$

where  $X_s$  is defined as

$$X_s = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \end{pmatrix}, \quad (2.4)$$

with

$$\xi_j = \frac{1}{2\sqrt{(2j+1)(2j-1)}}, \quad j = 1, \dots, s-1. \quad (2.5)$$

We now consider the matrix  $X_s(\alpha)$  obtained by perturbing (2.4) as follows:

$$X_s(\alpha) = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & \\ & & \xi_{s-1} + \alpha & 0 \end{pmatrix} = X_s + \alpha W_s, \quad (2.6)$$

where  $\alpha$  is a real parameter, and

$$W_s = \begin{pmatrix} 0 & 0 & & \\ 0 & 0 & \ddots & \\ & \ddots & \ddots & -1 \\ & & 1 & 0 \end{pmatrix}, \quad (2.7)$$

so that  $X_s(\alpha)$  is a rank two perturbation of  $X_s$ .

The family of methods  $y_1 = \Phi_h(y_0, \alpha)$  we are interested in, is defined by the following tableau:

$$\begin{array}{c|c} \begin{matrix} c_1 \\ \vdots \\ c_s \end{matrix} & \mathcal{A}(\alpha) \equiv \mathcal{P}X_s(\alpha)\mathcal{P}^{-1} \\ \hline & b_1 \dots b_s \end{array} \quad (2.8)$$

Therefore

$$\mathcal{A}(\alpha) = A + \alpha \mathcal{P}W_s\mathcal{P}^{-1}, \quad (2.9)$$

and hence  $\mathcal{A}(0) = A$ .

By exploiting Theorems 5.11 and 5.1 in [13, Chap. IV.5], we readily deduce that the symmetric method (2.8) has order  $2s - 2$  for any fixed  $\alpha \neq 0$ , and order  $2s$  when  $\alpha = 0$ .

We set

$$\omega = \begin{pmatrix} b_1 \\ \vdots \\ b_s \end{pmatrix}, \quad \Omega = \begin{pmatrix} b_1 & & \\ & \ddots & \\ & & b_s \end{pmatrix}, \quad e = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}. \quad (2.10)$$

**THEOREM 2.1.** *For any value of  $\alpha$ , the Runge-Kutta method defined in (2.8) is symplectic.*

**Proof** On the basis of [12, Theorem 4.3, page 192], we will prove the following sufficient condition for symplecticity:

$$\Omega \mathcal{A}(\alpha) + \mathcal{A}(\alpha)^T \Omega = \omega \omega^T.$$

Since the degree of the integrand functions in (2.1) does not exceed  $2s - 2$ , the orthogonality conditions may be equivalently posed in discrete form as

$$\sum_{k=1}^s b_k P_i(c_k) P_j(c_k) = \delta_{ij}, \quad i, j = 1, \dots, s,$$

or, in matrix notation,

$$\mathcal{P}^T \Omega P = I. \quad (2.11)$$

Considering that from (2.11) we get  $\mathcal{P}^{-1} = \mathcal{P}^T \Omega$ , from (2.9) we have that

$$\Omega \mathcal{A}(\alpha) + \mathcal{A}(\alpha)^T \Omega = \Omega A + A^T \Omega + \alpha \Omega \mathcal{P}(W_s + W_s^T) \mathcal{P}^T \Omega = \omega \omega^T \quad (2.12)$$

since the Gauss method is symplectic, and  $W_s$  is skew-symmetric so that  $W_s + W_s^T = 0$ .  $\square$

In the event that a value  $\alpha^* \equiv \alpha^*(y_0, h)$  for the parameter  $\alpha$  may be found such that the conservation condition  $H(y_1(\alpha)) = H(y_0)$  be satisfied, we can extrapolate from the parametric method (2.8) a symplectic scheme

$$y \mapsto \Phi_h(y, \alpha^*), \quad (2.13)$$

that provides energy conservation if evaluated at  $y_0$ . The existence of such an  $\alpha^*$  will be proved in Section 4. One important implication the use of (2.13) will guarantee is the conservation of all quadratic constant of motions associated with system (1.1). The fact that, in general,  $H(\Phi_h(y, \alpha^*)) \neq H(y)$ , explains the extent to which the energy conservation property of the new formulae must be interpreted. Summarizing, the new formulae, when applied to the initial value system (1.1) are able to define a numerical approximation of any high order, along which the Hamiltonian function and all quadratic first integrals of the system are precisely conserved.

**2.1. Generalizations.** The proof of Theorem 2.1 suggests how to extend the definition of the new formulae in order to get a family of methods depending on a set of parameters. Indeed, by looking at (2.12), in order to preserve symplecticity, it is sufficient to substitute to the matrix  $\alpha W_s$ , any skew-symmetric matrix  $\widetilde{W}_s$  of low rank, having non-null elements in the bottom-right corner so that, with respect to the Gauss method, the order is lowered as least as possible.

**THEOREM 2.2.** *Consider the  $s \times s$  matrix*

$$\widetilde{W}_s = \begin{pmatrix} 0 & \\ & V_r \end{pmatrix}$$

where  $V_r$  is any skew-symmetric matrix of dimension  $r + 1 < s$ . The Runge-Kutta method defined by the Butcher tableau

$$\begin{array}{c|cccc} c_1 & & & & \\ \vdots & & & & \\ c_s & & & & \\ \hline & b_1 & \dots & b_s \end{array} \quad \mathcal{A}(\alpha) \equiv \mathcal{P}(X_s + \widetilde{W}_s) \mathcal{P}^{-1} \quad (2.14)$$

in (2.8) is symplectic and has order  $p = 2(s - r)$ .

For example, a natural choice for the matrix  $\widetilde{W}_s$  is:

$$\widetilde{W}_s = \begin{pmatrix} 0 & 0 & & & \\ 0 & 0 & \ddots & & \\ & \ddots & \ddots & -\alpha_1 & \\ & & \alpha_1 & 0 & \ddots \\ & & & \ddots & \ddots & -\alpha_r \\ & & & & \alpha_r & 0 \end{pmatrix} \quad (2.15)$$

leading to a multi-parametric method depending on the  $r$  parameters  $\alpha_1, \dots, \alpha_r$ .

**3. Quasi-collocation conditions.** Condition (2.9) reveals the relation between the Butcher arrays associated with the new parametric method and the Gauss collocation method. In order not to lose generality, just in this subsection we assume to solve the generic problem  $\dot{y} = f(y)$ .

We wonder how the collocation conditions defining the Gauss methods are affected by the presence of the parameter  $\alpha$ . This is easily accomplished by expressing the coefficients of the perturbing matrix  $\mathcal{P}W_s\mathcal{P}^{-1}$  in terms of linear combinations of the integrals  $\int_0^{c_i} l_j(\tau)d\tau$ , where  $l_j(\tau)$  is the  $j$ th Lagrange polynomial defined on the abscissae  $c_1, \dots, c_s$ . Let  $\Gamma \equiv (\gamma_{ij})$  be the solution of the matrix linear system  $A\Gamma = \mathcal{P}W_s\mathcal{P}^{-1}$ , which means that (see (2.3))

$$\Gamma = \mathcal{P}X_s^{-1}W_s\mathcal{P}^{-1}. \quad (3.1)$$

The nonlinear system defining the block vector of the internal stages  $\{Y_i\}$  is

$$Y = e \otimes y_0 + h(A \otimes I)F(Y) + \alpha h(A\Gamma \otimes I)F(Y),$$

where  $e$  is the vector defined in (2.10), hereafter  $I$  is the identity matrix of dimension  $2m$ , and

$$Y = \begin{pmatrix} Y_1^T & \dots & Y_s^T \end{pmatrix}^T, \quad F(Y) = \begin{pmatrix} f(Y_1)^T & \dots & f(Y_s)^T \end{pmatrix}^T.$$

Therefore, the polynomial  $\sigma(t_0 + \tau h)$  of degree  $s$  that interpolates the stages  $Y_i$  at the abscissae  $c_i$ ,  $i = 1, \dots, s$ , is

$$\sigma(t_0 + \tau h) = y_0 + h \sum_{j=1}^s \int_0^\tau l_j(x)dx f(Y_j) + \alpha h \sum_{j=1}^s \left( \sum_{k=1}^s \gamma_{kj} \int_0^\tau l_k(x)dx \right) f(Y_j). \quad (3.2)$$

Differentiating (3.2) with respect to  $\tau$  gives

$$\dot{\sigma}(t_0 + \tau h) = \sum_{j=1}^s l_j(\tau) f(\sigma(t_0 + c_j h)) + \alpha \sum_{j=1}^s \left( \sum_{k=1}^s \gamma_{kj} l_k(\tau) \right) f(\sigma(t_0 + c_j h)). \quad (3.3)$$

Finally, evaluating (3.2) at  $\tau = 0$  and (3.3) at  $\tau = c_i$  yields

$$\begin{cases} \sigma(t_0) = y_0, \\ \dot{\sigma}(t_0 + c_i h) = f(\sigma(t_0 + c_i h)) + \alpha \sum_{j=1}^s \gamma_{ij} f(\sigma(t_0 + c_j h)), \end{cases} \quad i = 1, \dots, s. \quad (3.4)$$

For  $\alpha$  small, we can regard (3.4) as *quasi-collocation conditions*, since for  $\alpha = 0$  we recover the classical collocation conditions defining the Gauss method.

**3.1. Geometric interpretation.** Let us assume the existence of a quadratic first integral  $M(y)$  independent from  $H(y)$ : although this assumption is not strictly needed, it will somehow simplify the presentation of our argument.

Roughly speaking, for  $\alpha$  small, our *parametric* method may be interpreted as a symplectic perturbation of the Gauss method. Due to symplecticity of  $\Phi_h(\cdot, \alpha)$ , the parametric curve

$$\gamma \equiv \alpha \in D \mapsto y_1(\alpha) \in \mathbb{R}^{2m}, \quad (3.5)$$

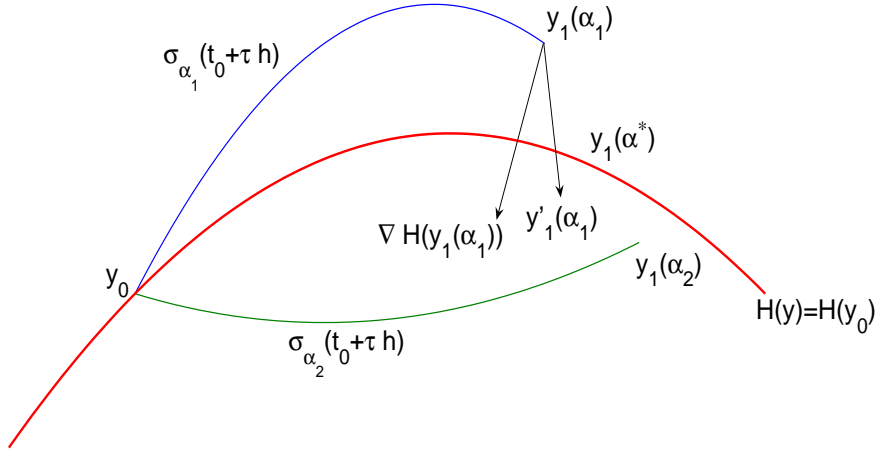


FIG. 3.1. A geometric interpretation of the parametric method (2.8). Two quasi-collocation polynomials  $\sigma_{\alpha_1}(t_0 + \tau h)$  and  $\sigma_{\alpha_2}(t_0 + \tau h)$  have as end-points the numerical solutions  $y_1(\alpha_1)$  and  $y_1(\alpha_2)$  which are  $O(h^{2s-1})$  close to the Hamiltonian since, for  $\alpha \neq 0$  the method has order  $2s-2$ . This means that the length of the arc of curve enclosed by the points  $y_1(\alpha_1)$  and  $y_1(\alpha_2)$  is  $O(h^{2s-1})$ . However, the parametric curve  $\gamma : \alpha \in [\alpha_1, \alpha_2] \mapsto y_1(\alpha)$  passes through  $y_1(0)$  which is at a distance  $O(h^{2s+1})$  from the manifold  $H(y) = H(y_0)$ , and there is a concrete possibility that this arc may intersect the manifold  $H(y) = H(y_0)$  at a point  $y_1(\alpha^*)$ .

where  $D$  is a given interval containing zero, will entirely lie in the manifold  $M(y) = M(y_0)$  and its length will be  $O(h^{2s-1})$ , since the method has order  $2s-2$ . However, the numerical solution produced by the Gauss method, namely  $y_1(0)$  will be  $O(h^{2s+1})$  close to the manifold  $H(y) = H(y_0)$ . Since the two manifolds contain the continuous solution, their intersection is nonempty and it is reasonable to expect that when  $\alpha$  ranges in  $D$ ,  $y_1(\alpha)$  can slide from a region where  $H(y_1(\alpha)) > H(y_0)$  to a region where  $H(y_1(\alpha)) < H(y_0)$ , thus producing a sign change in the scalar function

$$g(\alpha) = H(y_1(\alpha)) - H(y_0) \quad (3.6)$$

which, by continuity, will vanish at a point  $\alpha^*$ .

Obviously, similar arguments can be repeated for the multi-parameter version (2.14) of the method, where one has even more freedom in the choice of the parameters in the matrix  $\widetilde{W}_s$  defined in (2.15), in order to obtain the conservation of energy.<sup>2</sup>

**4. Theoretical existence results.** After defining the error function  $g(\alpha) = H(y_1(\alpha)) - H(y_0)$ , the nonlinear system, in the unknowns  $Y_1, \dots, Y_s$  and  $\alpha$ , that is to be solved at each step for getting energy conservation, reads

$$\begin{cases} Y = e \otimes y_0 + h(\mathcal{A}(\alpha) \otimes I)F(Y), \\ g(\alpha) = 0, \end{cases} \quad (4.1)$$

<sup>2</sup>We do not consider multi-parametric methods in the numerical results we present, since a single parameter suffices in getting the energy conservation property.

and its solvability is equivalent to the existence of the energy preserving method (2.13) we are looking for. After defining the vector function

$$G(h, y_1, \alpha) = \begin{pmatrix} y_1 - \Phi_h(y_0, \alpha) \\ H(y_1) - H(y_0) \end{pmatrix},$$

we see that system (4.1) is equivalent to  $G(h, y_1, \alpha) = 0$ . Of course  $G(0, y_1, \alpha) = 0$  for any value of  $\alpha$  and, in particular  $G(0, y_1, 0) = 0$ . The Jacobian of  $G$  with respect to the two variables  $y_1$  and  $\alpha$  reads

$$\frac{\partial G}{\partial(y_1, \alpha)}(h, y_1, \alpha) = \begin{pmatrix} I & \frac{\partial \Phi_h}{\partial \alpha}(y_0, \alpha) \\ \nabla^T H(y_1) & 0 \end{pmatrix},$$

where, as usual,  $I$  is the identity matrix of dimension  $2m$ . From (2.13) we see that  $\frac{\partial \Phi_h}{\partial \alpha}(y_0, \alpha)$  coincides with  $y'_1(\alpha)$  and, hence, with  $\sigma'_\alpha(t_0 + h)$ . Due to the consistency of the method, it follows that, for  $\alpha = 0$ ,  $\sigma'_\alpha(t_0 + h) \rightarrow J\nabla H(y_0)$  as  $h \rightarrow 0$ . Therefore

$$\frac{\partial G}{\partial(y_1, \alpha)}(0, y_1, 0) = \begin{pmatrix} I & J\nabla H(y_0) \\ \nabla^T H(y_0) & 0 \end{pmatrix}. \quad (4.2)$$

Unfortunately, the Jacobian matrix (4.2) is always singular. Consequently, the implicit function theorem (in its classical formulation) does not help in retrieving existence results of the solution of (4.1) when  $h$  is small. However, the rank of the matrix (4.2) is  $2m$  independently of the problem to be solved. This would suggest the use of the Lyapunov-Schmidt decomposition [22] that considers the restriction of the system to both the complement of the null space and the range of the Jacobian, to produce two systems to which the implicit function theorem applies.

In our case this approach is simplified in that the implicit function theorem assures the existence of a solution  $Y(\alpha)$  of the first system in (4.1) for all values of the parameter  $\alpha$  ranging in a closed interval containing the origin and  $|h| \leq h_0$ , with  $h_0$  small enough. Then  $y_1(\alpha) = y_0 + h(b^T \otimes I)Y(\alpha)$  is substituted into the second of (4.1) to produce the so called *bifurcation equation* in the unknown  $\alpha$ . When needed, we will explicitly write  $g(\alpha, h)$  or  $g(\alpha, h, y_0)$ , in place of  $g(\alpha)$ , to emphasize the dependence of the function  $g$  upon the stepsize  $h$ , that has to be treated as a parameter, and the state vector  $y_0$ .

Let us fix a vector  $y_0$  and look for solution curves of  $g(\alpha, h) = 0$  in the  $(h, \alpha)$  plane. Obviously  $g(\alpha, 0) = 0$  for any  $\alpha$ , which means that the axis  $h = 0$  is a solution curve of the bifurcation equation: of course, we are interested in the existence of a different solution curve  $\alpha^* = \alpha^*(h)$  passing through the origin. Since the gradient of  $g$  vanishes at  $(0, 0)$ , one has to compute the subsequent partial derivatives of  $g$  with respect to  $\alpha$  and  $h$ . However one verifies that  $\frac{\partial^2 g}{\partial h^2} = \frac{\partial^2 g}{\partial \alpha^2} = \frac{\partial^2 g}{\partial \alpha \partial h}$  evaluated at  $(0, 0)$  vanish as well, and this makes the computations even harder. For this reason, to address the question about the existence of a solution of (4.1), we make the following assumptions:

- (A<sub>1</sub>) the function  $g$  is analytical in a rectangle  $[-\bar{\alpha}, \bar{\alpha}] \times [-\bar{h}, \bar{h}]$  centered at the origin;
- (A<sub>2</sub>) let  $d$  be the order of the error in the Hamiltonian function associated with the Gauss method applied to the given Hamiltonian system (1.1) and the given state vector  $y_0$ , that is:

$$g(0, h) = H(y_1(0)) - H(y_0) = c_0 h^d + O(h^{d+1}), \quad (4.3)$$

with  $c_0 \neq 0$ . Then, we assume that for any fixed  $\alpha \neq 0$ ,

$$g(\alpha, h) = c(\alpha) h^{d-2} + O(h^{d-1}),$$



with  $c(\alpha) \neq 0$ .

REMARK 4.1. A couple of quick comments are in order before continuing. Excluding the case where the Hamiltonian  $H(q, p)$  is quadratic (which would imply  $g(\alpha, h) = 0$  for all  $\alpha$ ), the error in the numerical Hamiltonian function associated with the Gauss method is expected to behave as  $O(h^{2s+1})$ . Anyway, we cannot exclude a priori that special classes of problems or particular values for the state vector  $y_0$  may occur, for which the order of convergence may be even higher. This is why we have introduced the integer  $d$ : therefore such integer will be at least  $2s + 1$ . Moreover, we emphasize that the constant  $c_0$  and the function  $c(\alpha)$ , will depend on  $y_0$ . In conclusion, what we are assuming is that for the method (2.8), when  $\alpha$  is a given nonzero constant, the order of the error  $H(y_1(\alpha)) - H(y_0)$  is lowered by two units with respect to the underlying Gauss method of order  $2s$ , which is a quite natural requirement since such method has order  $2s - 2$ .

THEOREM 4.2. Under the assumptions  $(\mathcal{A}_1)$  and  $(\mathcal{A}_2)$ , there exists a function  $\alpha^* = \alpha^*(h)$ , defined in a neighborhood of the origin  $(-h_0, h_0)$ , such that:

- (i)  $g(\alpha^*(h), h) = 0$ , for all  $h \in (-h_0, h_0)$ ,
- (ii)  $\alpha^*(h) = \text{const} \cdot h^2 + O(h^3)$ .

Proof From  $(\mathcal{A}_1)$  and  $(\mathcal{A}_2)$  we obtain that the expansion of  $g$  around  $(0, 0)$  is:

$$g(\alpha, h) = \sum_{j=d}^{\infty} \frac{1}{j!} \frac{\partial^j g}{\partial h^j}(0, 0) h^j + \sum_{i=1}^{\infty} \sum_{j=d-2}^{\infty} \frac{1}{i!j!} \frac{\partial^{i+j} g}{\partial \alpha^i \partial h^j}(0, 0) h^j \alpha^i. \quad (4.4)$$

We are now in the right position to apply the implicit function theorem. We will look for a solution  $\alpha^* = \alpha^*(h)$  in the form  $\alpha^*(h) = \eta(h)h^2$ , where  $\eta(h)$  is a real-valued function of  $h$ . To this end, we consider the change of variable  $\alpha = \eta h^2$ , and insert it into (4.4) thus obtaining

$$\begin{aligned} g(\alpha, h) = & \frac{1}{d!} \frac{\partial^d g}{\partial h^d}(0, 0) h^d + \frac{1}{(d-2)!} \frac{\partial^{d-1} g}{\partial \alpha \partial h^{d-2}}(0, 0) h^d \eta \\ & + \frac{1}{(d-1)!} \frac{\partial^d g}{\partial \alpha \partial h^{d-1}}(0, 0) h^{d+1} \eta + \text{higher order terms.} \end{aligned} \quad (4.5)$$

Therefore, for  $h \neq 0$ ,  $g(\alpha, h) = 0$  is equivalent to  $\tilde{g}(\eta, h) = 0$ , where

$$\begin{aligned} \tilde{g}(\eta, h) = & \frac{1}{(d-1)d} \frac{\partial^d g}{\partial h^d}(0, 0) + \frac{\partial^{d-1} g}{\partial \alpha \partial h^{d-2}}(0, 0) \eta \\ & + \frac{1}{d-1} \frac{\partial^d g}{\partial \alpha \partial h^{d-1}}(0, 0) h \eta + \text{higher order terms.} \end{aligned} \quad (4.6)$$

By assumption  $(\mathcal{A}_2)$ , both  $\frac{\partial^d g}{\partial h^d}(0, 0)$  and  $\frac{\partial^{d-1} g}{\partial \alpha \partial h^{d-2}}(0, 0)$  are different from zero and hence the implicit function theorem assures the existence of a function  $\eta = \eta(h)$  such that  $\tilde{g}(\eta(h), h) = 0$ . The solution of  $g(\alpha, h) = 0$  for the variable  $\alpha$  will then be given by

$$\alpha^*(h) = \eta(h)h^2 = -\frac{1}{(d-1)d} \frac{\frac{\partial^d g}{\partial h^d}(0, 0)}{\frac{\partial^{d-1} g}{\partial \alpha \partial h^{d-2}}(0, 0)} h^2 + O(h^3), \quad (4.7)$$

and this completes the proof.  $\square$

By exploiting [17, Theorem 6.1.2], we see that the function  $\alpha^*(h)$  is analytic if the power series (4.4) is absolutely convergent for  $|h| \leq h_0$  and  $|\alpha| \leq \alpha_0$ . In any event, the function  $\alpha^*(h)$  is tangent

to the  $h$ -axis at the origin which means that a very small correction of the Gauss method is needed when the stepsize is small enough. As a matter of fact, the needed correction is so small that the resulting method (2.13) has indeed order  $2s$  instead of  $2s - 2$ , just as the Gauss method obtained by posing  $\alpha = 0$ . This is a consequence of the following result.

**THEOREM 4.3.** *Consider the parametric method (2.8) and suppose that the parameter  $\alpha$  is actually a function of the stepsize  $h$ , in such a way that  $\alpha(h) = O(h^2)$ . Then, the resulting method has order  $2s$ .*

**Proof** Let  $y_1(\alpha, h)$  be the solution computed by method (2.8) at time  $t_0 + h$ , starting at  $y_0 = y(t_0)$ , and consider its expansion with respect to the variable  $\alpha$ , in a neighborhood of zero:

$$y_1(\alpha, h) = y_1(0, h) + y'(\zeta_\alpha, h)\alpha.$$

We recall that  $y_1(0, h)$  is the numerical solution provided after a single step of the Gauss method and hence it is  $O(h^{2s+1})$  accurate while, for  $\alpha \neq 0$ ,  $y_1(\alpha, h)$  yields an approximation to the true solution of order  $2s - 1$ . This implies that  $y'(\zeta_\alpha, h)$  is  $O(h^{2s-1})$ . Consequently,

$$y_1(\alpha, h) - y(t_0 + h) = y_1(0, h) - y(t_0 + h) + y'(\zeta_\alpha, h)\alpha = O(h^{2s+1}) + \alpha O(h^{2s-1}),$$

from which we deduce that the error at the left hand side is  $O(h^{2s+1})$  if and only if  $\alpha = O(h^2)$ .  $\square$

Figure 4.1 reports the level curves of the function  $g(\alpha, h)$  in a neighborhood of the origin, for the Kepler problem described in Subsection 5.1 (the vector  $y_0$  has been chosen as in (5.3)). The tick lines in the plot correspond to the points  $(\alpha, h)$  in the plane where  $g$  vanish. This zero level set consists of the vertical axis  $h = 0$  and of the function  $\alpha^*(h)$ , which splits the region surrounding the origin into two adjacent subregions where the function  $g$  has clearly opposite sign. Despite the local character of the above existence result, we see that the branches of the function  $\alpha^*(h)$  extend away from the origin. Similar bifurcation diagrams may be traced starting at different values of  $y_0$  for all the test problems we have considered: this suggests that, in the spirit of the long-time simulation of dynamical systems, a quite large stepsize may be used during the numerical integration performed by method (2.13).

We end this section by providing a straightforward generalization of Theorem 4.2 to the case where the parameter  $\alpha$  is used to perturb a generic (not necessarily the last) element on the subdiagonal of the matrix  $X_s$ , and its symmetric.

**THEOREM 4.4.** *Consider the method (2.14) with  $\widetilde{W}_s$  as in (2.15) with  $\alpha_1 \equiv \alpha$  and  $\alpha_2 = \dots = \alpha_r = 0$ . We assume that assumption  $(A_1)$  and the following assumption (replacing  $(A_2)$ ) hold true:*

*$(A_2^r)$  let  $d$  be the order of the error in the Hamiltonian function associated with the Gauss method applied to the given Hamiltonian system (1.1) and the given state vector  $y_0$ . That is, (4.3) holds true. Then, we assume that for any fixed  $\alpha \neq 0$ ,*

$$g(\alpha, h) = c_r(\alpha)h^{d-2r} + O(h^{d-2r+1}),$$

*with  $c_r(\alpha) \neq 0$ .*

*Then, there exists a function  $\alpha^* = \alpha^*(h)$  defined in a neighborhood of the origin  $(-h_0, h_0)$  and such that:*

- (i)  $g(\alpha^*(h), h) = 0$ , for all  $h \in (-h_0, h_0)$ ,*
- (ii)  $\alpha^*(h) = \text{const} \cdot h^{2r} + O(h^{2r+1})$ .*

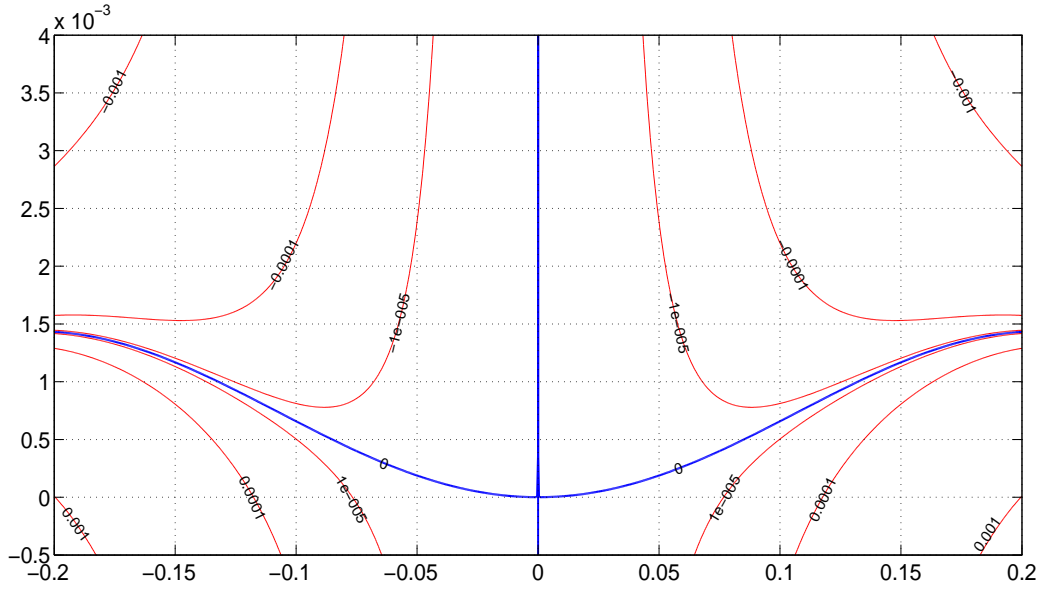


FIG. 4.1. Level curves in the plane  $(h, \alpha)$  of the function  $g(\alpha, h, y_0)$  associated with the method (2.8) of order four, for the Kepler problem (see Subsection 5.1), in a neighborhood of the origin:  $h \in [-0.2, 0, 2]$ ,  $\alpha \in [-0.5 \cdot 10^{-3}, 4 \cdot 10^{-3}]$ . Besides the  $\alpha$ -axis, a zero level curve tangent to the  $h$ -axis at the origin is visible. Such curve separates two regions around the origin where the function  $g$  has opposite sign. We notice that just a small correction of the Gauss method suffices to recover the energy preservation even for relatively large stepsizes.

The symplectic energy conserving method resulting from this choice of the parameter has order  $2s$ .

In the next section, we shall provide numerical evidence for the above presented results.

**5. Numerical tests.** In this section we present a few numerical tests showing the effectiveness of our approach. Method (2.13) and its generalization are implemented by solving, at each step, system (4.1). The efficient solution of such system will be the object of future studies; at present we adopt either one of the following techniques:

1. at each step, an interval  $[\alpha_1, \alpha_2]$  is detected such that  $g(\alpha_1)g(\alpha_2) < 0$ ; after that, a dichotomic search is implemented to locate  $\alpha^*$  within an error close to the machine precision;
2. the first (vector) equation in (4.1) is solved with  $\alpha_0 = 0$  (Gauss method) and  $\alpha_1 = ch^r$ , where  $c$  and  $r$  are suitable constants empirically estimated;<sup>3</sup> after that, a sequence  $\alpha_k$  is produced by solving the second (scalar) equation in (4.1) via the secant method.

In both cases, an outer iteration generating the sequence  $\alpha_k$  converging to  $\alpha^*$  is coupled with an inner iteration that determines the solution  $y_1(\alpha_k)$  starting from  $y_0$ . Such scheme is repeated at each step of integration.

The methods that we will consider in our experiments are: method (2.13) with  $s = 2$  (fourth order); method (2.13) with  $s = 3$  (sixth order); the sixth-order method described in Theorem 4.4 with  $s = 3$ , that is we insert a single perturbation parameter  $\alpha$  in the first (rather than in the second) subdiagonal element of the matrix  $X_3$ . In order to distinguish between these two methods

<sup>3</sup>For example see the last column in Table 5.1.

of order six, hereafter the latter will be referred to as “the order six method of the second type”.

**5.1. The Kepler problem.** In this problem, two bodies subject to Newton’s law of gravitation revolve about their center of mass, placed at the origin, in elliptic orbits in the  $(q_1, q_2)$ -plane. Assuming unitary masses and gravitational constant, the dynamics is described by the Hamiltonian function

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2} (p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}. \quad (5.1)$$

Besides the total energy  $H$ , a relevant first integral for the system is represented by the angular momentum

$$L(q_1, q_2, p_1, p_2) = q_1 p_2 - q_2 p_1. \quad (5.2)$$

Due to its symplecticity, the quadratic first integral (5.2) will be automatically conserved by method (2.8), for any choice of the parameter  $\alpha$ . On the other hand, we show that, at each step of integration, the parameter  $\alpha$  may be tuned in order to get energy conservation in the numerical solution.

As initial condition we choose

$$q_1(0) = 1 - e, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}}, \quad (5.3)$$

which confers an eccentricity equal to  $e$  on the orbit. Consequently,  $H(q, p) = -0.5$  and  $L(q, p) = \sqrt{1-e^2}$ . We set  $e = 0.6$  since, in this experiment, we are going to use constant stepsize (see [12, Sec. I.2.3]). More precisely, we solve problem (5.1) in the interval  $[t_0, T] = [0, 50]$  by the two-stages method (2.13) with the following set of stepsizes:  $h_i = 2^{-i}$ ,  $i = 1, \dots, 7$ . Figure 5.1 reports the errors in the Hamiltonian function  $H$  and in the angular momentum  $L$  of the numerical solutions generated by the method implemented with the intermediate stepsize  $h = 2^{-5}$ . These plots, which remain almost the same whatever is the stepsize considered in the given range, testify that the integration procedure performed by method (2.13) is indeed feasible and both energy and angular momentum preservation may be recovered in the discrete approximation of (1.1). For comparison purposes, we also report the same quantities for the Gauss methods of order 4 (corresponding to the choice  $\alpha = 0$  in (2.8)).

The second and third columns of Table 5.1 report the global error  $e(h_i) = |y_N(h_i) - y(T)|$ ,  $N = T/h_i$ , at the end point of the integration interval and the corresponding numerical order. According to Theorem (4.3), we see that the maximum order is preserved by method (2.13).

In Figure 5.2 the sequence  $\alpha_n^*$ , corresponding to the values of the parameter  $\alpha$  that at each step restore the conservation of the energy, are plotted for the case  $h = 2^{-5}$ . We consider  $\delta(h) = \max_n(\alpha_n^*) - \min_n(\alpha_n^*)$  as a measure of the total variability of the values of the sequence  $\{\alpha_n^*\}$ . Such quantity is reported in the fourth column of Table 5.1 for the values of the stepsize  $h_i$  used in this test. According to the result of Theorem 4.2, the last column in the table confirms that the dependence of  $\delta(h)$  on the stepsize  $h$  is of the form  $\delta = ch^2 + \text{h.o.t.}$ , with  $c \simeq 0.16$ .

**5.2. Test problem 2.** We consider the problem defined by the following polynomial Hamiltonian function:

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2} (p_1^2 + p_2^2) + (q_1^2 + q_2^2)^2. \quad (5.4)$$

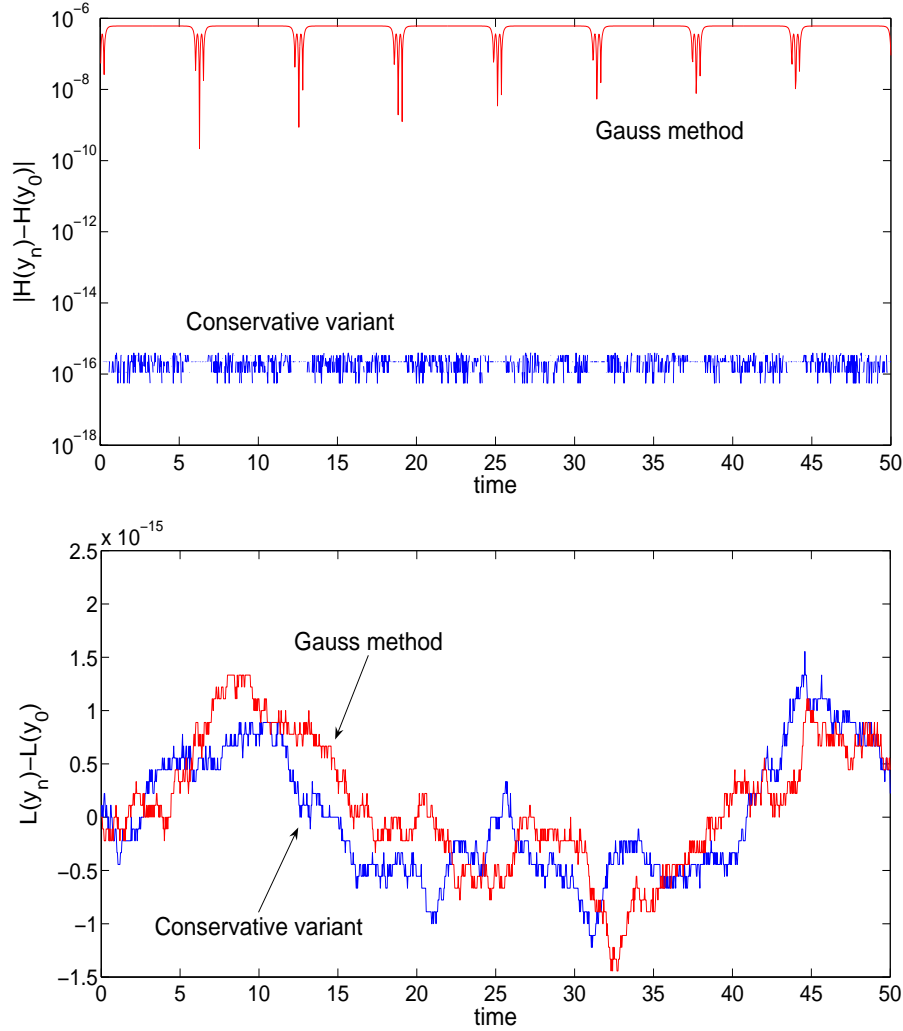


FIG. 5.1. *Upper picture: errors in the Hamiltonian function of the Kepler problem evaluated along the numerical solution generated by the Gauss method of order four and its conservative variant (method (2.13) with  $s = 2$ ). Bottom plot: error in the numerical angular momentum of the solution computed by the two methods. In both cases the stepsize used is  $h = 2^{-5}$ .*

This problem has been proposed in [19] as an example of a class of polynomial systems which, under suitable assumptions, admit an additional polynomial first integral  $F$  which is functionally independent from  $H$ . In this case, the additional (irreducible) first integral is

$$L(q_1, q_2, p_1, p_2) = q_1 p_2 - q_2 p_1. \quad (5.5)$$

The polynomial  $L$  being quadratic, we expect that our methods may preserve both  $H$  and  $L$ .<sup>4</sup>

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<sup>4</sup>Of course  $L$  may again be interpreted as the angular momentum of a mechanical system having (5.4) as Hamiltonian function.

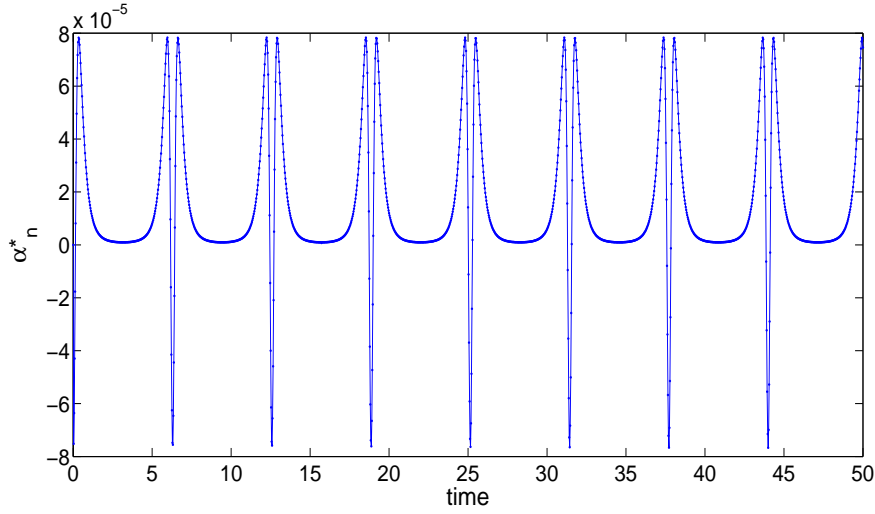


FIG. 5.2. Sequence of the values of the parameter  $\alpha^*$  in the method (2.13) with  $s = 2$  and  $h = 2^{-5}$ .

$h$	$e(h)$	order	$\delta(h)$	$\delta(h)/h^2$
$2^{-1}$	$2.62 \cdot 10^0$		$2.13 \cdot 10^{-2}$	$8.5374 \cdot 10^{-2}$
$2^{-2}$	$3.85 \cdot 10^{-1}$	2.763	$1.04 \cdot 10^{-2}$	$1.6700 \cdot 10^{-1}$
$2^{-3}$	$2.50 \cdot 10^{-2}$	3.945	$2.52 \cdot 10^{-3}$	$1.6185 \cdot 10^{-1}$
$2^{-4}$	$1.59 \cdot 10^{-3}$	3.970	$6.23 \cdot 10^{-4}$	$1.5951 \cdot 10^{-1}$
$2^{-5}$	$1.00 \cdot 10^{-4}$	3.991	$1.55 \cdot 10^{-4}$	$1.5878 \cdot 10^{-1}$
$2^{-6}$	$6.28 \cdot 10^{-6}$	3.997	$3.87 \cdot 10^{-5}$	$1.5862 \cdot 10^{-1}$
$2^{-7}$	$3.93 \cdot 10^{-7}$	3.999	$9.67 \cdot 10^{-6}$	$1.5856 \cdot 10^{-1}$

TABLE 5.1

Performance of the order four method (2.13) applied to the Kepler problem. The global error at  $T = 50$  (second column), and the corresponding order obtained via the formula  $\log_2(e(h_i)/e(h_{i+1}))$ , indicate that the perturbations introduced in the Gauss collocation conditions (see (3.4)) are small enough that the order 4 of the Gauss method with two stages is conserved by its energy preserving variant. The last two columns give a measure of the perturbations and of the rate they tend to zero as  $h \rightarrow 0$ . The quantity  $\delta(h)$  is the amplitude of the minimum interval that encloses all the values  $\alpha_n^*$  for the given stepsize  $h$  and in the given integration interval. Hence the last column confirms what proved in Theorem 4.2, namely that the perturbations are  $O(h^2)$ .

We have solved problem (5.4) by means of two methods of order six ( $s = 3$ ): method (2.13), and the order six method of the second type, described in Theorem 4.4.

Figure 5.3 reports the errors in the Hamiltonian function  $H$  and in the quadratic first integral  $L$  of the numerical solutions generated by the latter method implemented with the intermediate stepsize  $h = 2^{-3}$ . For comparison purposes, we also report the same quantities for the Gauss methods of order six.

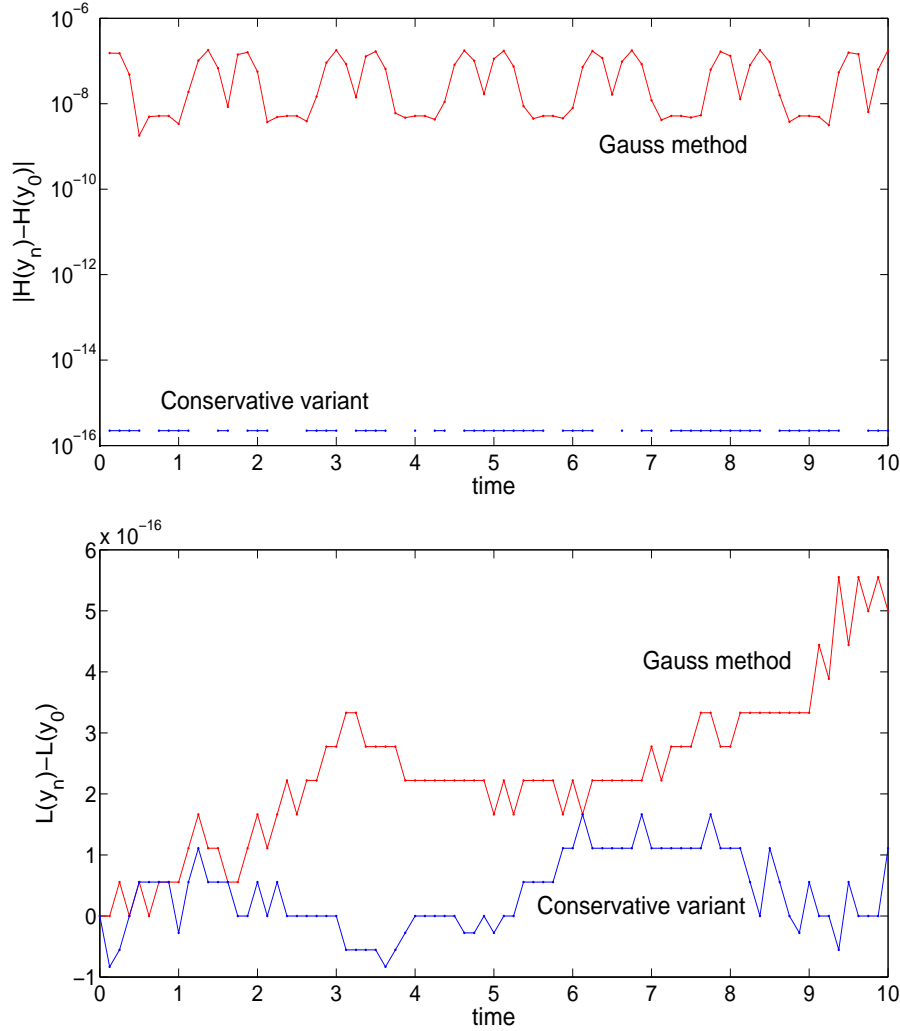


FIG. 5.3. Upper picture: errors in the Hamiltonian function of test problem 2 evaluated along the numerical solution generated by the Gauss method of order six and its conservative variant of the second type. Bottom plot: error in the quadratic first integral (5.5) of the solution computed by the two methods. In both cases the stepsize used is  $h = 2^{-3}$ .

Tables 5.2 and 5.3 are the analogues of Table 5.1 for these two methods: we see that both methods achieve order six but, while in the former  $\alpha^*(h) = O(h^2)$ , in the latter  $\alpha^*(h) = O(h^4)$  consistently with Theorems 4.2, 4.3, and 4.4.

**5.3. The Hénon-Heiles problem.** The Hénon-Heiles equation originates from a problem in Celestial Mechanics describing the motion of a star under the action of a gravitational potential of a galaxy which is assumed time-independent and with an axis of symmetry (the  $z$ -axis) (see [14] and references therein). The main question related to this model was to state the existence of a third first integral, beside the total energy and the angular momentum. By exploiting the symmetry of

$h$	$e(h)$	order	$\delta(h)$	$\delta(h)/h^2$
$2^{-1}$	$2.17 \cdot 10^{-2}$		$1.59 \cdot 10^{-2}$	$6.37 \cdot 10^{-2}$
$2^{-2}$	$4.59 \cdot 10^{-4}$	5.562	$3.99 \cdot 10^{-3}$	$6.39 \cdot 10^{-2}$
$2^{-3}$	$7.77 \cdot 10^{-6}$	5.884	$9.99 \cdot 10^{-4}$	$6.40 \cdot 10^{-2}$
$2^{-4}$	$1.24 \cdot 10^{-7}$	5.970	$2.53 \cdot 10^{-4}$	$6.48 \cdot 10^{-2}$
$2^{-5}$	$1.94 \cdot 10^{-9}$	5.992	$6.33 \cdot 10^{-5}$	$6.49 \cdot 10^{-2}$
$2^{-6}$	$3.05 \cdot 10^{-11}$	5.994	$1.59 \cdot 10^{-5}$	$6.51 \cdot 10^{-2}$

TABLE 5.2

Performance of method (2.13) of order six applied to problem (5.4). The reported quantities are the analogues of the ones presented in Table 5.1.

$h$	$e(h)$	order	$\delta(h)$	$\delta(h)/h^4$
$2^{-1}$	$4.91 \cdot 10^{-2}$		$5.59 \cdot 10^{-2}$	0.895
$2^{-2}$	$1.46 \cdot 10^{-2}$	1.753	$1.51 \cdot 10^{-2}$	3.87
$2^{-3}$	$1.84 \cdot 10^{-4}$	6.304	$4.92 \cdot 10^{-4}$	2.01
$2^{-4}$	$3.23 \cdot 10^{-6}$	5.836	$4.07 \cdot 10^{-5}$	2.66
$2^{-5}$	$4.73 \cdot 10^{-8}$	6.091	$2.30 \cdot 10^{-6}$	2.41
$2^{-6}$	$7.03 \cdot 10^{-10}$	6.074	$1.50 \cdot 10^{-7}$	2.51

TABLE 5.3

Performance of the sixth-order method of the second kind applied to problem (5.4).

the system and the conservation of the angular momentum, Hénon and Heiles reduced from three (cylindrical coordinates) to two (planar coordinates) the degrees of freedom, thus showing that the problem was equivalent to the study of the motion of a particle in a plane subject to an arbitrary potential  $U(q_1, q_2)$ :

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2}(p_1^2 + p_2^2) + U(q_1, q_2). \quad (5.6)$$

In particular, for their experiments they chose

$$U(q_1, q_2) = \frac{1}{2}(q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3}q_2^3, \quad (5.7)$$

which makes the Hamiltonian function a polynomial of degree three. When  $U(q_1, q_2)$  approaches the value  $\frac{1}{6}$ , the level curves of  $U$  tend to an equilateral triangle, whose vertices are saddle points of  $U$  (see Figure 5.4). This vertices have coordinates  $P_1 = (0, 1)$ ,  $P_2 = (-\frac{\sqrt{3}}{2}, -\frac{1}{2})$  and  $P_3 = (\frac{\sqrt{3}}{2}, -\frac{1}{2})$ .

Since  $U$  in (5.6) has no symmetry in general, we cannot consider the angular momentum as an invariant anymore, so that the only known first integral is the total energy represented by (5.6)



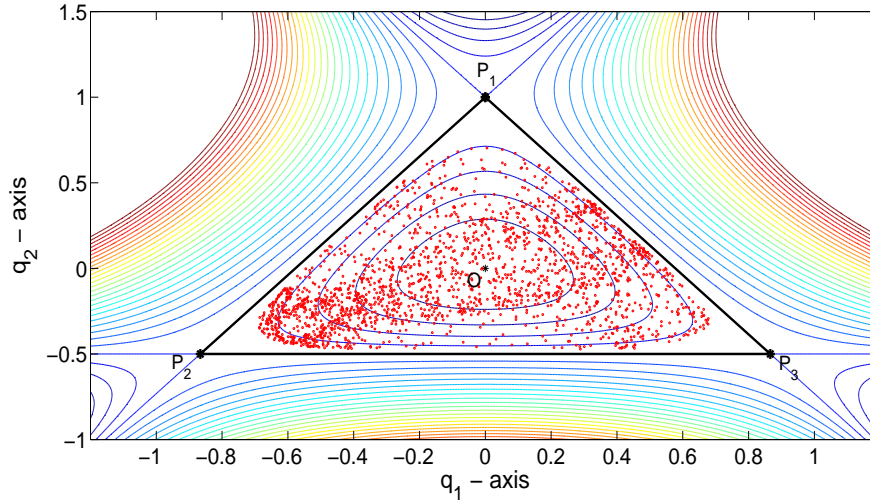


FIG. 5.4. Level curves of the potential  $U(q_1, q_2)$  of the Hénon-Heiles problem (see (5.7)). The origin  $O$  is a stable equilibrium point, whose domain of stability contains the equilateral triangle having as vertices the saddle points  $P_1$ ,  $P_2$ , and  $P_3$ , provided that the total energy does not exceed the value  $\frac{1}{6}$ . Inside the triangle, a numerical trajectory (small dots) computed by the sixth-order method of the second type with stepsize  $h = 0.25$  and in the time interval  $[0, 500]$ , is traced: its total energy is 0.15.

itself, and the question is whether or not a second integral does exist. Hénon and Heiles conducted a series of tests with the aim of giving a numerical evidence of the existence of such integral for moderate values of the energy  $H$ , and of the appearance of chaotic behavior when  $H$  becomes larger than a critical value: it is believed that for values of  $H$  in the interval  $(\frac{1}{8}, \frac{1}{6})$  this second first integral does not exist (see also [12, Section I3]).

We consider the initial point  $P_0 = (q_{10}, q_{20}, p_{10}, p_{20}) = (0, 0, \sqrt{\frac{3}{10}}, 0)$  which confers on the system a total energy  $H = 0.15 \in (\frac{1}{8}, \frac{1}{6})$ . Therefore the orbit originating from  $P_0$  will never abandon the triangle for any value of the time  $t$ . We have integrated problem (5.6) in the time interval  $[0, 500]$  with stepsize  $h = 0.25$  by using the Gauss method of order six and its conservative variant of the second type. Figure 5.5 shows the errors in the Hamiltonian function  $H$  in both cases.

**6. Conclusions.** We have defined a new class of symmetric and symplectic one-step methods of any high order that, under somewhat weak assumptions, are capable to compute a numerical solution along which the Hamiltonian function is precisely conserved. This feature has been realized by first introducing a symplectic parametric perturbation of the Gauss method, and then by selecting the parameter, at each step of the integration procedure, in order to get energy conservation. A relevant implication of the symplectic nature of each formula is the conservation of all quadratic first integrals associated to the system. With the help of the implicit function theorem, we have shown that not only do these methods exist, but that the correction required on the Gauss method is so small that the order of convergence of this latter method is preserved by its conservative variant. A few test problems have been reported to confirm the theoretical results presented, and to show the effectiveness of the new formulae.

This approach opens a number of interesting routes of investigation. First of all, if preferred,

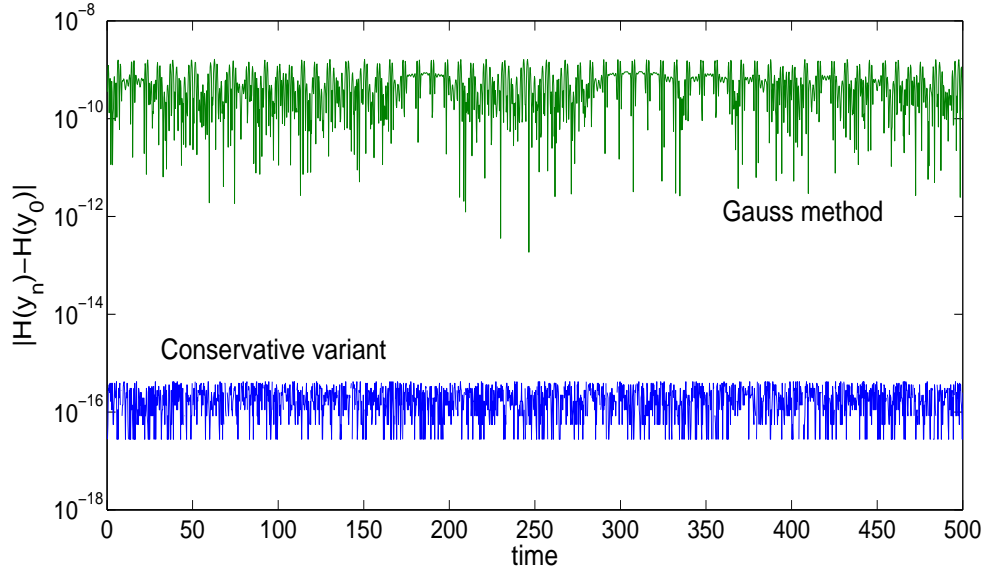


FIG. 5.5. Errors in the Hamiltonian function (5.6)-(5.7) evaluated along the numerical solution generated by the Gauss method of order six and its conservative variant of the second type. Stepsize:  $h = 0.25$ ; time interval:  $[0, 500]$ ; initial condition  $(q_{10}, q_{20}, p_{10}, p_{20}) = (0, 0, \sqrt{\frac{3}{10}}, 0)$ .

the parameter could be selected in such a way to impose the conservation of other non quadratic first integrals different from the Hamiltonian function itself. More generally, the multi-parametric generalization introduced suggests the possibility of choosing the free parameters in order to impose the conservation of a number of functionally independent first integrals possessed by the continuous problem. Last but not least, the idea of considering symplectic corrections of the Gauss method could be in principle extended to other classes of symplectic methods known in the literature. The above described lines of investigation, as well as the efficient solution of the nonlinear systems arising from the conservation requirements, will be the subject of future researches.

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